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Calculating the Gibbs energy of hydrogen bonding for proton acceptors with a solvent in methanol solutions

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Abstract

We propose a method for calculating the Gibbs energies of hydrogen bonding of solutes with associated solvents via the thermodynamic analysis of experimental values of solvation Gibbs energies. The method is applied to solutions of different proton acceptors in methanol. It is shown that the contribution of hydrogen bonding processes to the solvation Gibbs energy in methanol is in most cases very different in magnitude from the formation Gibbs energy of equimolar complexes of the solute and methanol. We demonstrate the need to include the contributions from solvophobic effects in investigating intermolecular interactions in associated solvents by means of thermodynamic data. © 2011 Pleiades Publishing, Ltd.

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Keywords

associated solvents, Gibbs energy, hydrogen bonding, methanol solutions, solvation, solvophobic effects